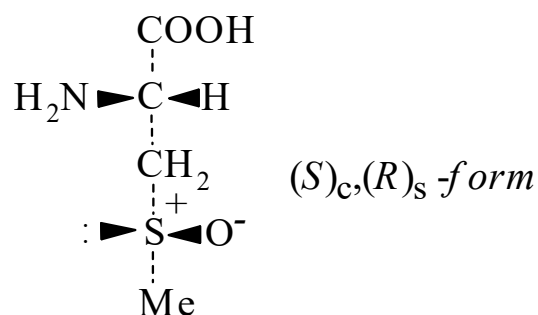




>>Entry Name: **S-Methylcysteine sulfoxide**

ENTRY UNDER REVIEW

Synonym(s): 3-(Methylsulfinyl)alanine, 9Cl. **Methiin**



Molecular Formula: C₄H₉NO₃S

Molecular Weight: 151.186

Accurate Mass: 151.030314

Percentage Composition: C 31.78%; H 6.00%; N 9.26%; O 31.75%; S 21.21%

>>Variant: (S)_c(R)_s-form

CAS Registry Number: 3226-62-8

Molecular Formula: C₄H₉NO₃S

Molecular Weight: 151.186

Accurate Mass: 151.030314

Percentage Composition: C 31.78%; H 6.00%; N 9.26%; O 31.75%; S 21.21%

Melting Point: Mp 165 dec.°

Optical Rotation: [α]_D -202 (c, 0.4 in H₂O)

>>Derivative: *N*-Ac

Molecular Formula: C₆H₁₁NO₄S

Molecular Weight: 193.223

Accurate Mass: 193.040879

Percentage Composition: C 37.30%; H 5.74%; N 7.25%; O 33.12%; S 16.60%

Melting Point: Mp 168-169° (as dicyclohexylammonium salt)

Optical Rotation: [α]_D -251 (c, 1.5 in H₂O)

>>Variant: (S)_c(S)_s-form

CAS Registry Number: 32726-14-0

Extra CAS Registry Numbers(s): 6853-87-8

Molecular Formula: C₄H₉NO₃S

Molecular Weight: 151.186

Accurate Mass: 151.030314

Percentage Composition: C 31.78%; H 6.00%; N 9.26%; O 31.75%; S 21.21%

Biological Source: Constit. of onion (*Allium cepa*) other *Allium* spp. and *Brassica* spp.

Melting Point: Mp 163 dec.°

Optical Rotation: [α]_D +204 (c, 0.4 in H₂O)

>>Derivative: *N*-Ac

Molecular Formula: C₆H₁₁NO₄S

Molecular Weight: 193.223

Accurate Mass: 193.040879

Percentage Composition: C 37.30%; H 5.74%; N 7.25%; O 33.12%; S 16.60%

Melting Point: Mp 166-167° (as dicyclohexylammonium salt)

Optical Rotation: [α]_D +138 (c, 1.5 in H₂O)

References:

- Barnsley, E.A., *Tetrahedron*, 1968, **24**, 3747, (*synth, abs config*)
Meese, C.O. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1990, **323**, 957
Meese, C.O. *et al.*, *Z. Naturforsch., C*, 1990, **45**, 1171, (*pmr*)
Kubec, R. *et al.*, *J. Agric. Food Chem.*, 2000, **48**, 428-433, (*occur*)